Charge injection and transport in organic light emitting diodes

J. Campbell Scott, Luisa Bozano,
IBM Almaden Research Center, San Jose CA
Beat Ruhstaller, Heike Riel and Walter Riess
IBM Zurich Research Lab, Rueschlikon, Switzerland
and Sue A. Carter
Physics Department, UC Santa Cruz

The physical processes underlying the operation of organic light emitting diodes are, in general, well understood. They are charge injection from the metallic electrodes into the organic layers, charge transport across these layers, trapping and detrapping, electron-hole recombination and exciton emission. The detailed description of device performance requires consideration of all these processes in a self-consistent manner, and in all real cases requires numerical modeling. This talk gives a summary of our development of a predictive model, using a continuum electrostatic approach, for the steady state and transient behavior of multilayer OLEDs.

Since all the charge-related phenomena depend on electric field, it is necessary first to know the electric field distribution across the OLED device. There are three contributions to the electric field. First, the built-in field due to the difference in workfunctions of the anode and cathode (modified by the presence of dipole layers at the electrode interfaces) can be determined by photocurrent or electroabsorption measurements. The built-in voltage and, second, the externally applied voltage are divided across the structure, according to the dielectric constants of each layer. The third contribution is the space-charge field which arises from the distribution of electrons and holes in each layer. Since it cannot be measured directly, its self-consistent determination is the crux of the calculational problem.

Independent experiments in single layer samples, with electrode pairs chosen to inject only one sign of carrier, provide considerable information about the transport of electrons and holes in the materials of interest. The charge mobility exhibits the field and temperature dependence typical of hopping in amorphous organic materials, and in many materials both holes and electrons are sufficiently mobile that bipolar currents must be accounted for. Diffusion constants are more difficult to determine experimentally, but our numerical simulations show that their absolute values have little effect on, at least, the steady-state behavior. In the dynamic response, diffusive charge spreading is difficult to distinguish from trapping and detrapping.

Charge injection from the electrodes has been shown to depend upon the mobility in the amorphous organic transport layers. Although the injection of an individual electron or hole is a tunneling event from the delocalized states of the metal to the localized states in the organic, the net injection current is well described as a thermionic process, with a dependence on electric field dominated by the barrier-lowering Schottky effect.

Charge injection from one organic layer to another at internal organic interfaces is less well studied experimentally. In our model, we rely on prior theoretical understanding of the charge hopping process, where the difference in energies between the source and target sites enters as an Arrhenius dependence in the hopping rate.

In keeping with the hopping nature of transport in organic materials, the bimolecular recombination of electrons and holes is described as a Langevin process, i.e. the rate is given by the sum of the electron and hole mobilities.

Consideration of all the phenomena in the preceding paragraphs permits a self-consistent and time-dependent solution for the electric field profile and charge distributions throughout the OLED structure as exemplified in Fig. 1. The rate of exciton creation is proportional to the product of electron and hole densities. The emission rate is modified from that given by the bulk fluorescence lifetime because of the proximity of the metallic electrodes relative to the wavelength, and the orientation of the transition dipole moment - so-called microcavity effects. Lastly, for a complete description of the device efficiency, one must consider the fate of the emitted photon. Does it propagate at an angle which permits it to leave the device in a "useful" direction, or is it internally reflected and guided to the edges of the high refractive index layers.

It is apparent from the foregoing discussion that a complete model of any real OLED device structure requires the knowledge of many materials parameters: electrode workfunctions, interface dipole moments (vacuum level offsets), energies of the transport levels (offset from the HOMO and LUMO levels by polarization energies) and field and temperature dependent mobilities of electrons and holes in each organic layer. Trap level distribution, either extrinsic or deliberately introduced in the form of emissive dopant dyes, must also be taken into account. There are very few cases in which all of these parameters are known. Nevertheless, by making reasonable "guestimates" we have been able to compare the predictions of the model with real experimental data. Several examples will be given. The results are in good quantitative agreement and confirm that the essential physics of device operation are as described. They provide guidance in optimizing OLED structure and composition.

For a more complete description of this work, see B. Ruhstaller et al. *J. Appl. Phys.* **89**, 4575 (2001) and references therein.

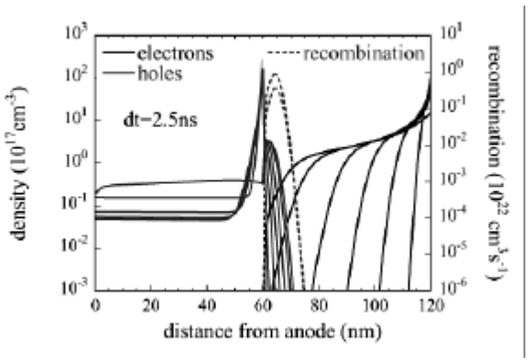

Figure 1. Time dependent response (at 2.5 ns intervals) of the electron, hole and recombination densities in a bilayer device following a 10 V step in voltage. Parameters used are appropriate for a TPD hole transport layer and an Alq3 electron transport/emission layer.